

# Study of the low-temperature behavior of a disordered antiferromagnet with random fields by the parallel-tempering method

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The parallel-tempering method has been applied to numerically study the thermodynamic behavior of a three-dimensional disordered antiferromagnetic Ising model with random fields at spin concentrations corresponding to regions of both weak and strong structural disorder. An analysis of the low-temperature behavior of the model convincingly shows that in the case of a weakly disordered samples there is realized an antiferromagnetic ordered state, while in the region of strong structural disorder the effects of random magnetic fields lead to the realization of a new phase state of the system with a complex domain structure consisting of antiferromagnetic and ferromagnetic domains separated by regions of a spin-glass phase and characterized by a spinglass ground state.

## I. INTRODUCTION

Studying the critical behavior of disordered systems with quenched structural defects is of a great theoretical and experimental interest since the majority of real solids contain quenched structural defects whose presence influences their thermodynamic characteristics and, in particular, substantially affects the behavior of the systems during phase transitions. It is known that the effect of quenched impurities manifests itself in the form of random disturbances of the local temperature in ferro and antiferromagnetic systems in the absence of an external magnetic field or in the form of random magnetic fields in antiferromagnetic systems in a uniform magnetic field.

The investigations performed showed that in the first case the presence of quenched nonmagnetic impurity atoms changes the properties of only anisotropic Ising like magnets

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in phase transitions in which the heat capacity in the purely uniform state diverges at a critical temperature. In the opposite case of magnets described by the XY model or by the isotropic Heisenberg model, the presence of an impurity does not affect their behavior during phase transitions. The critical properties of the disordered Ising model has recently been studied in numerous works (see references in [1]). For the dilute Ising-like systems, good agreement was obtained between the theoretical calculations and the results of experiments and computer simulation by the Monte Carlo method. An opposite situation is observed for the magnetic systems with a disorder of the random magnetic field type. In spite of numerous studies, which began since 1975 when this type of disorder was described for the first time [2], only scarce reliable information on the behavior of these systems exists at present [3]. In particular, the nature of the phase transition in the three-dimensional Ising model with random fields still remains unexplained, and the theoretical results obtained contradict the experimental data. The comparison of theoretical predictions with the results of experimental studies is hindered by the difficulties of achieving the equilibrium state in such systems because of their anomalously slow relaxation properties. According to some data, this is a first-order transition [4, 5] up to very low values of random fields; according to other, this is a second-order transition [6, 7].

For describing the influence of random fields on the behavior of magnetic systems, two qualitatively equivalent models, namely, the ferromagnetic random-field Ising model (RFIM) [8, 9] and the disordered antiferromagnetic Ising model in an external uniform field (DAFF) [10] are used. The real magnetic systems with the effects of random fields are antiferromagnets with quenched impurities of nonmagnetic atoms; in the behavior of these systems, effects of a ferromagnetic interaction of next-nearest atoms manifest themselves along with the antiferromagnetic interaction of nearestneighbor atoms. The structure of an antiferromagnet can be represented as several ferromagnetic sublattices inserted into each other in such a way that the total magnetization of the antiferromagnet remains equal to zero despite the fact that at a temperature lower than the Néel point there occurs a magnetic ordering within each ferromagnetic sublattice. As examples of two-sublattice antiferromagnets, NiO, MnO, Fe<sub>2</sub>O<sub>3</sub>, MnF<sub>2</sub>, and some other can be mentioned. As the examples of the realization of disordered systems with random magnetic fields, uniaxial Ising-like antiferromagnets such as MnF<sub>2</sub> and FeF<sub>2</sub> with impurities of Zn atoms in an external magnetic field can be taken [11].

In [12, 13], we for the first time showed, using Monte Carlo computer simulation of the thermodynamic behavior of the disordered antiferromagnetic Ising model with effects of random magnetic fields, that, in weakly disordered systems with a spin concentration higher than the threshold for impurity percolation, a second-order phase transition from the paramagnetic into the antiferromagnetic state is realized. In strongly disordered systems with a spin concentration lower than this threshold value, a first-order transition from the paramagnetic into a mixed state, which is characterized by a complex domain structure consisting of antiferromagnetic and ferromagnetic domains separated by regions of a spinglass phase, occurs in the system. It was shown that, with a reduction in the spin concentrations and an increase in the magnitude of the external magnetic field, a decrease in the number and sizes of antiferromagnetic domains occurs in the system, and an increase in the number and sizes of ferromagnetic domains along with a reduction of the relative volume of the spin-glass phase is observed. It is shown that in this region of spin concentrations the effects of random magnetic fields lead to a change from an antiferromagnetic ground state to a spin-glass state.

In this work, we consider the same antiferromagnetic Ising model (with a spin concentration  $p = 0.5$  corresponding to the region of strong structural disordering) as in [12, 13]. The aim is to obtain an additional confirmation of the existence in such systems of a spin-glass ground state and of a complex domain structure by the realization and application, for its numerical study, of the algorithm of the parallel-tempering method which was developed specially for studying the thermodynamics of spin glasses. To compare the results obtained, we also investigated the model at  $p = 0.9$  corresponding to the region of weak disorder.

## II. MODEL

The disordered two-sublattice antiferromagnetic Ising model was defined as a system of spins with a concentration  $p$  connected with  $N = pL^3$  sites of a cubic lattice with periodic boundary conditions. The Hamiltonian of the model under consideration has the form

$$\mathcal{H} = J_1 \sum_{i,j} p_i p_j \sigma_i \sigma_j + J_2 \sum_{i,k} p_i p_k \sigma_i \sigma_k + \mu h \sum_i p_i \sigma_i, \quad (1)$$

where  $\sigma_i = \pm 1$ ,  $\mu$  is the Bohr magneton,  $J_1 = 1$  and  $J_2 = -1/2$  characterize the antiferromagnetic interaction of spins with nearest neighbors and their ferromagnetic interaction with next-nearest neighbors, respectively; and  $h$  is the intensity of a uniform magnetic field.

The random variables  $p_i$  and  $p_j$  are described by the distribution function

$$P(p_i) = p\delta(p_i - 1) + (1 - p)\delta(p_i) \quad (2)$$

and characterize the quenched nonmagnetic impurity atoms distributed over the lattice sites (empty sites).

The simulation of statistical properties of this model made it possible to determine thermodynamic values such as the total magnetization

$$M = \frac{1}{pL^3} \left[ \left\langle \sum_i p_i \sigma_i \right\rangle \right], \quad (3)$$

the staggered magnetization  $M_{stg} = M_1 - M_2$  ( $M_1$  and  $M_2$  – are the magnetizations of the sublattices), and the spin-glass order parameter

$$q_{\alpha,\beta} = \frac{1}{pL^3} \left[ \sum_i \langle p_i \sigma_i \rangle_{(\alpha)} \langle p_i \sigma_i \rangle_{(\beta)} \right], \quad (4)$$

where the exponents  $\alpha$  and  $\beta$  characterize different replicas of the disordered system that are simulated simultaneously at one and the same temperature and have different initial configurations. In expressions (3) and (4), the angular brackets designate statistical averaging realized for each impurity configuration of the system, and the brackets mean averaging over different impurity configurations.

The quantities  $M$ ,  $M_{stg}$ , and  $q_{\alpha,\beta}$ , characterize different types of magnetic ordering of a strongly disordered system that can appear in it in the low-temperature phase. Along with these magnetic thermodynamic quantities, measurements of the heat capacity as a thermal characteristic of occurring phase transformations in the system were realized.

### III. PARALLEL-TEMPERING METHOD

As is known, the spin-glass state is characterized by the presence of a large number of metastable energy states separated by potential barriers. The number of metastable states exponentially grows with increasing number of spins, which strongly complicates the numerical simulation of such systems. In spin glasses, there is a problem of reaching an equilibrium state because of the existence of high energy barriers which separate local energy minima. At sufficiently low temperatures, the system can never leave a local energy minimum even if the corresponding state is globally unstable. This feature

makes impossible obtaining physical characteristics for the magnetic materials which contain, as in our case, a spin-glass phase when using standard Monte Carlo algorithms. There arises a need for an improvement or a modification of the algorithms used for simulation. One of the algorithms which made it possible to solve this problem became the parallel-temperature algorithm [14].

The parallel-tempering method is an extension of the usual Metropolis algorithm. The optimization consists in the addition to the Metropolis algorithm of a second Markov chain in the temperature parameter  $\beta = J_1/T$ . The new distribution law is in this case written as

$$P(\{\sigma\}, \{\beta_\alpha\}) \sim \exp(-\beta_\alpha H(\{\sigma\}) + g_\alpha), \quad (5)$$

$g_\alpha$  is a certain constant. To each  $\beta_\alpha$  there corresponds its own  $g_\alpha$ . The probability of changing the dynamic parameter  $\beta_\alpha$  will obey an  $\exp(-S)$ , law, where

$$S = (\beta'_\alpha - \beta_\alpha)H(\{\sigma\}) + (g'_\alpha - g_\alpha). \quad (6)$$

In the case of the simultaneous simulation of the replicas of the system for each  $\beta_\alpha$  with  $\alpha = 0 \dots N$ , the change in the temperature can depend only on the nearest values of  $\alpha$ ; i.e., we have  $\beta'_\alpha = \beta_{\alpha \pm 1}$ . The probability of a transition between the states that are determined by adjacent temperatures will be written as  $\exp(-\Delta S)$ , where  $\Delta S$  is assigned by the expression

$$\Delta S = S' - S = (E_{\beta_\alpha} - E_{\beta_{\alpha+1}})(\beta_{\alpha+1} - \beta_\alpha). \quad (7)$$

According to this algorithm, the temperature of the system can in the process of simulation both decrease (annealing of the system) and increase, which makes it possible for the system to surmount high potential barriers.

The basic criterion for the application of the parallel-tempering method is the overlap of the energy-distribution functions of the replicas of the system for adjacent temperatures (Fig. 1). Since the energy variance approaches zero with decreasing temperature, the selection of equidistant temperatures is not justified; the interval between adjacent temperatures

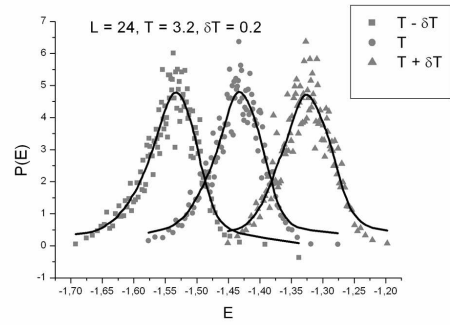


FIG. 1: Overlap of energy distributions for adjacent replicas.

$\delta T = T_{\alpha+1} - T_\alpha$  also should decrease. This dependence leads to additional difficulties upon the simulation of the behavior of these systems in the region of low temperatures, since the initial maximum temperature of simulation  $T_N$  should be sufficiently large to surmount the potential barriers which separate the local energy minima. Meanwhile, the number of replicas of the system (at different temperatures) considered in simulation must ensure the mechanism of temperature exchange. Under the conditions of a finite number of the simulated replicas, which is limited by the computational resources of the researcher, it is necessary to solve the problem of an optimum choice of the number of temperatures to be considered. Theoretically, the most optimum selection of temperatures, according to [15, 16], is such at which the probability of a transition of the replica to a new temperature is constant for the entire set of the replicas:

$$P(E_\alpha, \beta_\alpha \rightarrow E_{\alpha+1}, \beta_{\alpha+1}) = \min[1, \exp(-\Delta S)] \simeq \text{const}. \quad (8)$$

As an optimum sequence of temperatures, we can use the geometric progression  $T_{\alpha+1}/T_\alpha = \text{const}$  with:

$$T_\alpha = T_0 R^\alpha (\alpha = 0..N), \quad (9)$$

where  $R = \sqrt[N]{T_N/T_0}$ .

The choice of the temperature sequence in this form ensures the fulfillment of equality (8). The optimum value of the probability of the replica transition to a new temperature upon the realization of the parallel-tempering algorithm was determined [17] to be  $P \simeq 0.23$ .

However, in contrast to the Ising spin glasses, in which the temperature of transition into the spin-glass state is  $T_f/J \approx 1$ , in the dilute antiferromagnetic Ising model with the effects of random magnetic fields at a spin concentration  $p = 0.5$  the temperature of the phase transition into the mixed state is  $T_m \approx 5$  in the units of exchange integral  $J_1$ . As a result, the application of the parallel-tempering method to the simulation of such a system requires the use of a considerably wider temperature range. Thus, to guarantee obtaining a stable initial equilibrium state from which it is better to perform simulation, the initial maximum temperature  $T_N$  must be selected to be considerably higher than the temperature  $T_{\text{mix}}$ ; only after this it is possible to investigate the phase transition into the mixed state near  $T_{\text{mix}}$  in the vicinity of which there already appears a set of metastable states with an extremely slow dynamics of establishing equilibrium. On the other hand, for studying the asymptotic approach to the ground spin-glass state of the system it is desirable that the minimum

temperature  $T_0$  be as close as possible to  $T = 0$ . All this imposes new restrictions on the realization of the parallel-tempering algorithm for studying disordered antiferromagnets and for the selection of the sequence of temperatures for the replicas to be simulated.

Note also that for the realization of the condition of the equal probability of the temperature exchange between the adjacent replicas it is necessary to have information on the temperature dependence of the energy of the system  $E(T)$ ; for this reason, the procedure of finding an optimum set of temperature points requires a preliminary simulation of the system. As the first approximation, a sequence of temperatures in the form of a geometric progression (9) can be chosen. The subsequent simulation of the system for the selected temperatures gives an idea about the  $E(T)$  dependence, though also only in the first approximation. At the next step, a new set of temperatures  $\beta'_\alpha$  is determined according to condition (8) to yield

$$(E(\beta'_\alpha) - E(\beta'_{\alpha+1})) (\beta'_{\alpha+1} - \beta'_\alpha) \simeq \text{const} . \quad (10)$$

The new set of temperatures obtained in this case specifies new (more optimum) parameters for the simulation of the disordered system. In turn, the thus obtained replica-temperature distribution is also an approximation (second-order), which can be used for the subsequent iterative search for the optimum set of temperatures.

The inconvenience of this approach is the need to, each time anew, conduct the complete simulation of the system at each step of the search for an optimum sequence of temperatures. Nevertheless, this approach makes it possible to most effectively use the parallel-tempering algorithm in conducting numerical experiments on studying the low-temperature properties of spin-glass states.

#### IV. RESULTS AND DISCUSSION

In this work, we consider the antiferromagnetic Ising model with a spin concentration  $p = 0.5$  (corresponding to the region of strong disordering) and a magnetic field  $h = 2$ . The simulation was conducted for a wide set of values of the linear dimensions of the cubic lattice ( $L = 8, 16, 24, 32$ , and  $40$ ).

For determining the temperature of the phase transition in the system and the intervals of existence of different phase states, we studied the temperature behavior of the heat capacity

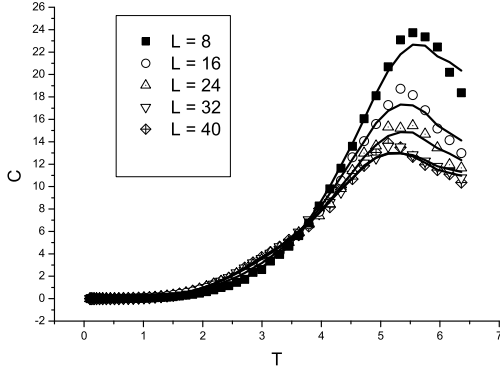


FIG. 2: Temperature dependence of the heat capacity  $C$  for systems with a spin concentration  $p = 0.50$  and linear sizes  $L = 8, 16, 24, 32$ , and  $40$ .

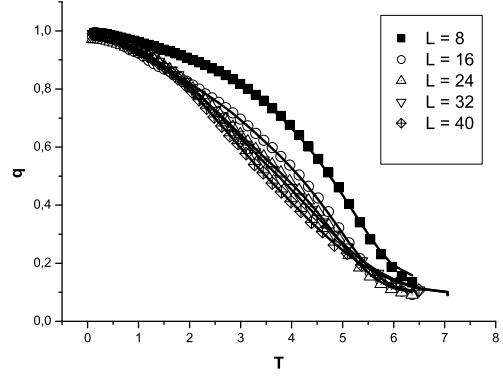


FIG. 3: Temperature dependence of the spin-glass order parameter  $q$  for the systems with a spin concentration  $p = 0.50$  and linear sizes  $L = 8, 16, 24, 32$ , and  $40$ .

of the system (Fig. 2) for the lattices of the above-indicated dimensions. It is evident that in the temperature interval of  $T = 4.56.5$  there is observed an anomalous increase in the heat capacity, which indicates the existence of a phase transition in the system. The size-dependent changes in the behavior of the heat capacity indicate the suppression of the energy fluctuations in the system in comparison with the typical second-order phase transitions into the antiferromagnetic state, and the bend in the temperature dependence  $C(T)$  at  $T_{\text{mix}} = 5.13$  for the lattice with  $L_{\text{max}} = 40$  is typical of the phase transition in spin glasses [3].

For obtaining equilibrium magnetic characteristics of the system, the initial states were selected in the paramagnetic phase. This choice is caused by the fact that, because of the presence of metastable states near the transition temperature and in the entire low-temperature phase, there arises a problem of reaching equilibrium initial configurations. The initial states obtained were used in the realization of the parallel-tempering method. Within the framework of this method, the initial set of temperatures was selected according to formula (9). The temperature dependence of the energy  $E(T)$  obtained in the simulation was used for refining the temperatures  $\beta_\alpha$  according to the principle of the equal probability of transition between adjacent temperatures. To achieve the equilibrium state of the system at each temperature,  $10^4$  Monte Carlo steps were used for the relaxation, with the rejection of half initial configurations.



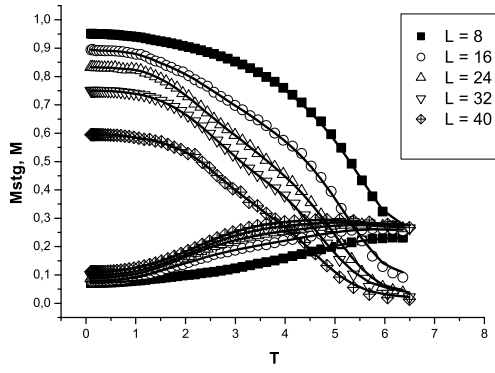


FIG. 4: Temperature dependence of the staggered ( $M_{\text{stg}}$ , upper curves) and total ( $M$ , lower curves) magnetizations for systems with a spin concentration  $p = 0.50$  and linear sizes  $L = 8, 16, 24, 32$ , and  $40$ .

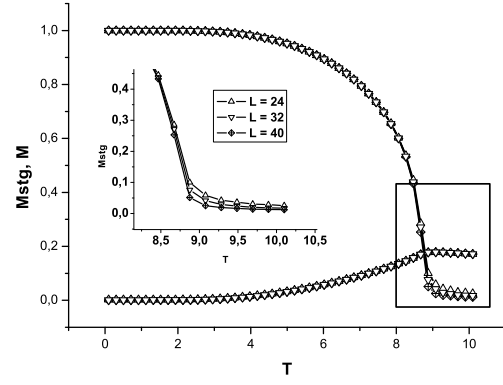


FIG. 5: Temperature dependence of staggered ( $M_{\text{stg}}$ , upper curves) and total ( $M$ , lower curves) magnetizations for systems with a spin concentration  $p = 0.90$  and linear sizes  $L = 24, 32$ , and  $40$ . In the inset, the temperature range of phase transition is shown for  $M_{\text{stg}}$ .

Figures 3-4 display the temperature dependences obtained for the staggered ( $M_{\text{stg}}$ ) and total ( $M$ ) magnetizations and spin-glass order parameter ( $q$ ) for the lattices with linear dimensions from  $L = 8$  to  $L = 40$  averaged over 100 different impurity configurations. It is seen from the figures that all the values measured demonstrate a noticeable dependence on the sizes of the system. The strongest dependence on  $L$  is characteristic of the staggered magnetization, which for the systems of small sizes determines the prevailing magnetic ordering of antiferromagnetic nature; the spin-glass order parameter in this case appears as a secondary parameter of ordering and repeats the temperature dependence of the staggered magnetization. The strong decrease in  $M_{\text{stg}}$  with increasing  $L$  at noticeably smaller changes in the spin-glass order parameter indicates the predominance of spin-glass ordering in the system with  $L > 24$  and the appearance, in the low-temperature phase, of a mixed phase state consisting of antiferromagnetic and ferromagnetic domains surrounded by a spin-glass phase. Note that at a temperature  $T_{\text{mix}} = 5.13$  the temperature dependence of the total magnetization for the lattice with  $L = 40$  reaches a maximum with a subsequent characteristic decrease in  $M(T)$  in the high-temperature region, as was observed in [13]. The results obtained indicate that, in the limit of  $L \rightarrow \infty$  and  $T \rightarrow 0$ , a spin-glass ground state is

realized in the system.

To compare the observed features of the behavior of the magnetic characteristics of the model in the region of strong structural disorder with the behavior of analogous characteristics in the region of weak dilution, we carried out an analogous study for the samples with a spin concentration  $p = 0.9$ . Figure 5 displays the temperature dependences of the staggered ( $M_{\text{stg}}$ ) and total ( $M$ ) magnetizations on the linear dimensions of the lattice  $L = 24, 32$ , and 40. It is evident that no size dependence of these characteristics is observed in the low-temperature phase, except for the temperature range close to the critical temperature  $T_c = 8.73$ . The temperature behavior of  $M_{\text{stg}}$  clearly indicates the existence of an antiferromagnetic ordering in the system with an the antiferromagnetic ground state under above conditions.

To confirm the existence of a domain structure in the mixed phase state of the strongly disordered antiferromagnet with random fields, we realized, within the framework of the statistical parallel-tempering method, a study of the temperature dependence of the local values of magnetic characteristics for cubic blocks of size  $b = 5, 10$ , and 20 into which the lattice under consideration (with a maximum size  $L = 40$ ) was divided. These dependences are shown in Figs. 6-8; solid curves correspond to the depen-

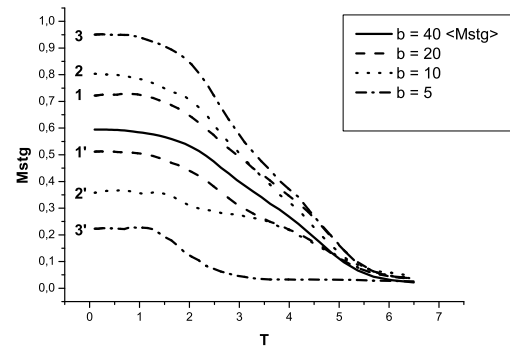


FIG. 6: Temperature dependence of the local values of the staggered magnetization  $M_{\text{stg}}$  for blocks with sizes  $b = 5, 10$ , and 20.

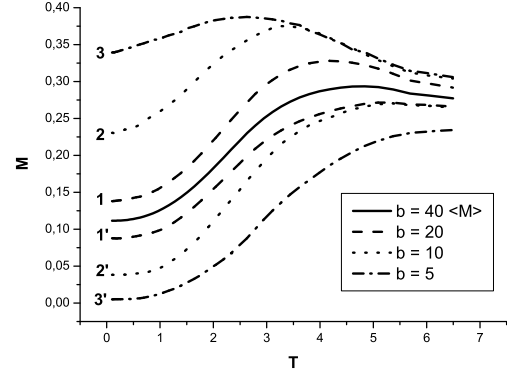


FIG. 7: Temperature dependence of the local values of the total magnetization  $M$  for blocks with sizes  $b = 5, 10$ , and 20.

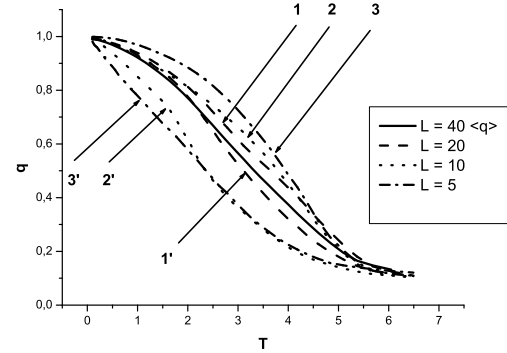


FIG. 8: Temperature dependence of the local values of the spin-glass order parameter  $q$  for blocks with sizes  $b = 5, 10$ , and 20.

solid curves correspond to the depen-

dence of the average values of  $M_{\text{stg}}(T)$ ,  $M(T)$ , and  $q(T)$  for the entire lattice with  $L = 40$ ; curves 1 and 1', 2 and 2', and 3 and 3' correspond to minimum and maximum values of these values for the blocks with  $b = 5, 10$ , and  $20$ , respectively. An analysis of these figures and the data on the entire totality of blocks shows that as the temperature decreases, the sizes of typical antiferromagnetic domains decrease from  $l_a \simeq 20$  to  $l_a \simeq 10$ , and the sizes of ferromagnetic domains, from  $l_f \simeq 10$  to  $l_f \simeq 5$  with an increase in the volume of the spin-glass phase, until at  $T = 0$  there is realized a spin-glass ground state.

## Conclusions

Thus, by applying the numerical parallel-tempering method for studying the low-temperature behavior of the three-dimensional disordered antiferromagnetic model with random magnetic fields, it was clearly shown that in weakly disordered systems there is realized an antiferromagnetic ordered state, whereas in the region of strong structural disorder the effects of random magnetic fields lead to the realization of a new phase state in the system, which is characterized by a complex domain structure consisting of antiferromagnetic and ferromagnetic domains separated by regions of a spin-glass phase with the realization of a spin-glass ground state.

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